Thermodynamics of Solitonic Matter Waves in a Toroidal Trap

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We investigate the thermodynamic properties of a Bose-Einstein condensate with negative scattering length confined in a toroidal trapping potential. By numerically solving the coupled Gross-Pitaevskii and Bogoliubov-de Gennes equations, we study the phase transition from the uniform state to the symmetry-breaking state characterized by a bright-soliton condensate and a localized thermal cloud. In the localized regime three states with a finite condensate fraction are present: the thermodynamically stable localized state, a metastable localized state and also a metastable uniform state. Remarkably, the presence of the stable localized state strongly increases the critical temperature of Bose-Einstein condensation.

In recent experiments a repulsive Bose-Einstein condensate (BEC) has been produced and studied in a quasi one-dimensional (1D) ring [1,2]. These experiments and also previous experimental investigations with cold atoms in torodial traps [3] are important steps to achieve ultra-high precision sensors with atom interferometry (see for instance [4]). The case of an attractive BEC in a ring has not yet been experimentally investigated but appears very interesting: a quantum phase transition from an azimuthally uniform condensate to a bright soliton has been predicted [5,6]. Dynamically stable multi-peak bright solitons may also appear [7].

In this paper we investigate the effect of temperature on the uniform-to-localized phase transition by solving the Gross-Pitaevskii equation (GPE) of the macroscopic wave function of the Bose condensate and the Bogoliubov-de Gennes equations for the quantum depletion and the thermal cloud. We show that, for a fixed number N of atoms, the uniform solution always exists but it is thermodynamically stable only up to a critical interaction strength which depends on the temperature. Above this critical interaction strength both condensate and thermal cloud become localized. In addition, we determine the finite-temperature phase-diagram of the system for a sample of alkali-metal atoms in a ring. Our results are relevant not only for the physics of cold atoms but also for the nonlinear science of solitons. In fact, a mixture of condensed and non condensed attractive particles [8] correspond to incoherent solitons of light in Kerr media [9].

We consider a Bose gas with negative scattering length ($a_s < 0$) confined in a toroidal potential and model the transverse confinement with a harmonic potential of frequency $\omega_\perp$. The two characteristic lengths of the toroidal trap are the azimuthal radius R and the transverse harmonic length $a_\perp = (\hbar/(m\omega_\perp))^{1/2}$. To avoid the confinement-induced resonance at $|a_s| \simeq a_\perp$ [10] we impose that $|a_s| \ll a_\perp$ [11]. At low temperature T and with

a finite number N of atoms, in the Bose gas there is the thermal cloud but also the BEC. Under the condition $R \gg a_\perp$ the azimuthal wavefunction $\phi(z)$ of the BEC in the ring satisfies the 1D non-polynomial Schrödinger equation (NPSE) [7,12]

$$\left[-\frac{\hbar^2}{2m}\partial_z^2 + \mu(n_0(z)) \right] \phi(z) = \bar{\mu}\, \phi(z) \, , \qquad (1)$$

where $z = R\theta$ is the azimuthal coordinate with θ the azimuthal angle. This equation has been deduced from the 3D GPE by using a Gaussian transverse wave function with a density-dependent width and neglecting curvature effects [7,12]. The non-polynomial term $\mu(n_0(z))$ is a function of the BEC density $n_0(z) = N_0|\phi(z)|^2$ and it is given by $\mu = \partial\mathcal{E}/\partial n_0$, where $\mathcal{E} = \hbar\omega_\perp\, n_0(1+2a_s n_0)^{1/2}$ and $a_s < 0$ is the 3D s-wave scattering length [7]. The wave function $\phi(z)$ is normalized to one and satisfies the condition of periodicity $\phi(z+L) = \phi(z)$, where $L = 2\pi R$. The chemical potential $\bar{\mu}$ is fixed by the normalization condition $\int |\phi(z)|^2 dz = 1$. Quantum and thermal depletions of the BEC are obtained by solving the Bogoliubov-de Gennes (BdG) equations [13] for the quasi-particle amplitudes $u_\alpha(z)$ and $v_\alpha(z)$, given by

$$\mathcal{L} \left(\begin{array}{c} u_\alpha(z) \\ v_\alpha(z) \end{array} \right) = \epsilon_\alpha \left(\begin{array}{c} u_\alpha(z) \\ v_\alpha(z) \end{array} \right) \, , \qquad (2)$$

where ϵ_α are the energies of quasi-particle excitations and the operator $\mathcal{L}$ is

$$\mathcal{L} = \left(\begin{array}{cc} -\frac{\hbar^2}{2m}\partial_z^2 - \bar{\mu} + \frac{\partial(n_0\mu)}{\partial n_0} & N_0\phi^2\frac{\partial\mu}{\partial n_0} \\ -N_0(\phi^*)^2\frac{\partial\mu}{\partial n_0} & \frac{\hbar^2}{2m}\partial_z^2 + \bar{\mu} - \frac{\partial(n_0\mu)}{\partial n_0} \end{array} \right) \, . \quad (3)$$

The local density of the quantum depletion reads $n_{out}(z) = \sum_\alpha |v_\alpha(z)|^2$, while the thermal local density is $n_T(z) = \sum_\alpha \left(|u_\alpha(z)|^2 + |v_\alpha(z)|^2 \right) \bar{n}_\alpha$, where $\bar{n}_\alpha = (\exp(\epsilon_\alpha/k_B T) - 1)^{-1}$ are the Bose numbers of occupation for the non-interacting quasi-particles, k_B is the

Boltzmann constant and T is the absolute temperature of the thermal cloud. The number $\tilde{N}$ of non-condensed atoms is thus given by $\tilde{N} = N_{out} + N_T$, where $N_{out} = \int n_{out}(z)dz$ and $N_T = \int n_T(z)dz$. In the weak-coupling limit, where $a_s n_0 \ll 1$, the energy density $\mathcal{E}$ becomes $\mathcal{E} = \hbar\omega_\perp n_0 + \hbar\omega_\perp a_s n_0^2$, the NPSE (1) reduces to the familiar 1D GPE [7] and the BdG equations (2,3) reduce to the BdG equations of the strictly 1D problem. Note that the Eqs. (1) and (2,3) could be improved by taking into account Popov and Beliaev corrections, which are usually not negligible only when the condensed fraction is very small [14].

In our approach, by fixing the total number $N = N_0 + \tilde{N}$ of atoms and the temperature T, the equilibrium configurations are found from the Helmholtz free energy [13]

$$F = E_0 + \tilde{E} + \bar{\mu}(N - N_0) - TS , \qquad (4)$$

where

$$E_0 = N_0 \int \left[-\frac{\hbar^2}{2m}\phi^*(z)\partial_z^2\phi(z) + \mathcal{E}(n_0(z)) \right] dz \qquad (5)$$

is the BEC energy. The out-of-condensate energy $\tilde{E}$ and entropy S are instead given by

$$\tilde{E} = \sum_\alpha \epsilon_\alpha \left[\bar{n}_\alpha - \int |v_\alpha(z)|^2 dz \right] \qquad (6)$$

$$S = -k_B \sum_\alpha [\bar{n}_\alpha \log(\bar{n}_\alpha) - (1 + \bar{n}_\alpha)\log(1 + \bar{n}_\alpha)] . \qquad (7)$$

The solution of the 1D GPE with periodic boundary conditions is known analytically [5]: it is uniform for $0 < \gamma N_0 < \pi^2 a_\perp/L$, with $\gamma = 2|a_s|/a_\perp$ the interatomic strength, and becomes localized for $\gamma N_0 > \pi^2 a_\perp/L$. By using the NPSE we find that the transition strength approaches the 1D GPE one for large L [7]. The main difference between 1D GPE and NPSE is that the NPSE correctly gives the collapse of the localized solution for $\gamma N_0 > 4/3$, while the 1D GPE does not predict collapse [7]. It is important to observe that the uniform-to-localized transition depends on N_0 and only implicitly on $N = N_0 + N_{out} + N_T$. We shall show that, for a fixed number N of atoms, the uniform solution exists for any value of the interatomic strength γ but it is thermodynamically stable only below a critical strength γ_c. Above γ_c the stable state is a localized solution that minimizes the free energy.

The BdG equations (2,3) are easily solved if $\phi(z)$ is uniform: $\phi(z) = 1/\sqrt{L}$. In this case the quasi-particle amplitudes $u_k(z) = \bar{u}_k e^{ikz}$ and $v_k(z) = \bar{v}_k e^{-ikz}$ are plane waves and the wave vector k is quantized: $k = (2\pi/L)j$, with j an integer number. When $\phi(z)$ is not uniform, one must numerically solve Eq. (1) and Eqs. (2,3). We use a finite-difference space discretization and diagonalize the matrix associated to the operator $\mathcal{L}$ of Eq. (3). In

our calculations we use various matrix dimensions up to 4000×4000. The numerical procedure is discussed in [15]. In our approach the transverse excitations do not contribute to the thermodynamics: this assumption is reasonable only if the system is quasi-1D.
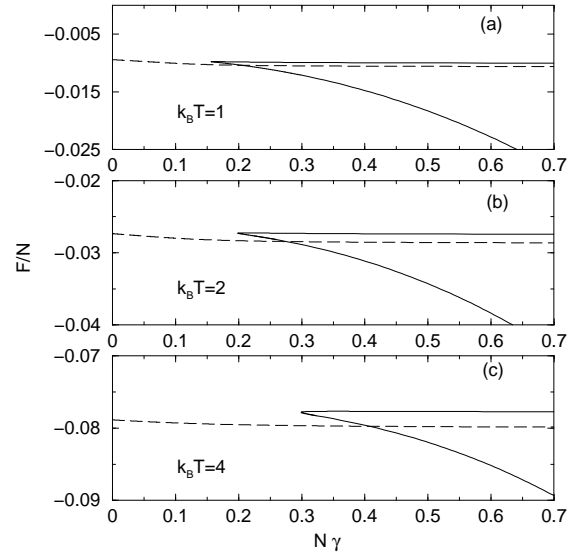

FIG. 1 Free energy F as a function of the scaled interatomic strength $\gamma = 2|a_s|/a_\perp$ for an attractive Bose gas of $N = 10^4$ atoms in a toroidal trap with $L/a_\perp = 100$. Dashed line: uniform solution. Solid line: localized solutions. The energies F and $k_B T$ are in units of $\hbar\omega_\perp$.

In Fig. 1 we plot the results of our numerical calculations of the free energy F as a function of the scaled interatomic strength $\gamma = 2|a_s|/a_\perp$ for increasing values of the temperature T. We choose $N = 10^4$ atoms and a toroidal geometry with $L/a_\perp = 100$. While the uniform solution (dashed line) exists for any strength γ, the localized solution (solid line) exists only above a critical strength γ_e. As expected, at $T \simeq 0$ we find $\gamma_c \simeq \pi^2 a_\perp/L = 0.0987$. For a given γ ($\gamma > \gamma_e$) there are two localized states: one is thermodynamically stable (lower solid line) and the other is metastable (upper solid line). The metastability is guaranteed by the Bogoliubov eigenvalues being real. At very-low temperature, see panel (a) of Fig. 1, for $\gamma > \gamma_e$ the solid line of the metastable localized solution is very close to the dashed line of the metastable uniform solution. At higher temperature, see panels (b) and (c) of Fig. 1, the free energy of the metastable localized solution, but also the free energy of the stable one at small $\gamma > \gamma_e$, is higher than the free energy of the uniform solution. The strength γ_c at which the dashed line crosses the lower solid line determines the point where the first-order transition takes place. At $T \simeq 0$ we find that $\gamma_c \simeq \gamma_e$. The strength γ_c grows with the temperature T but in general γ_c does not coincide with the strength γ_e at which the localized solutions appear. Thus, at finite temperature, for $0 < \gamma < \gamma_e$ there is only the stable uniform

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state; for $\gamma_e < \gamma < \gamma_c$ there are two metastable localized states and the stable uniform state; for $\gamma > \gamma_c$ the stable state is one of the two localized state while the other localized state and the uniform state are metastable.
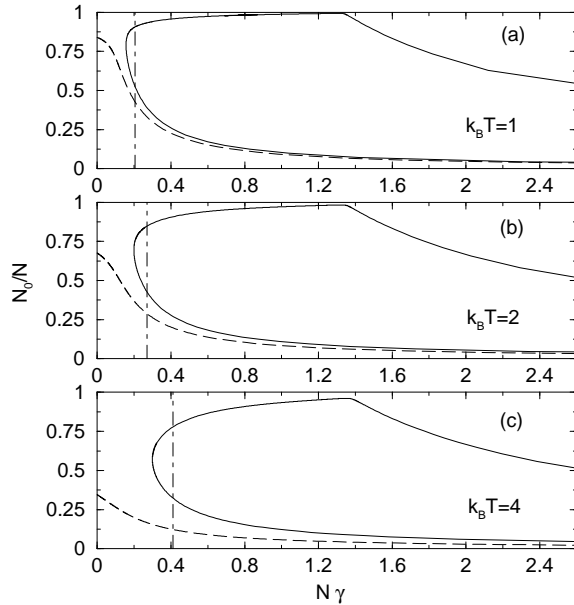

FIG. 2 Condensate fraction N_0/N as a function of the scaled interatomic strength $\gamma = 2|a_s|/a_\perp$ for $N = 10^4$ atoms with $L/a_\perp = 100$. Dashed line: uniform solution. Solid line: localized solutions. The vertical dot-dashed line indicates the strength $N\gamma_c$ at which the uniform-to-localized phase transition takes place.

A coherent bright soliton and a thermal cloud coexist in the stable state, as in the metastable localized state. This is clearly illustrated in Fig. 2 where we plot the condensate fraction N_0/N as a function of γ for different temperatures. At low temperature, see panel (a) of Fig. 2, the uniform state (dashed line) is a quasi-pure BEC for $0 < \gamma < \gamma_e$. For $\gamma > \gamma_e$ the condensate fraction of the uniform state quickly decreases. At low temperature the uniform-to-localized phase transition does not produce a relevant quantum depletion N_{out}/N at the transition point. This result is obtained with a fixed number of atoms ($N = 10^4$). We have verified that by fixing N_0 instead of N (as done in [5]) the condensate fraction N_0/N goes to zero for $\gamma N_0 \simeq \pi^2 a_\perp/L$.

At higher temperature, see panels (b) and (c) of Fig. 2, BEC and non-condensate component coexist also in the uniform state. Fig. 2 shows that the condensate fraction of the localized states is higher than the condensate fraction of the uniform state. Remarkably, at the transition strength γ_c there is a sizeable jump in the condensate fraction. Moreover, for the stable localized state the ratio N_0/N initially grows by increasing the interatomic strength. As previously discussed, the BEC soliton of the localized state will collapse at $\gamma N_0 \simeq 4/3$,

but the true collapse is avoided by populating the out-of-condensate cloud with $\tilde{N} = N - N_0$ atoms for $N\gamma > 4/3$. We have verified that in the stable localized state the number N_0 of condensed atoms is always very close to the collapse value $4/(3\gamma)$ and, for a fixed γ, the number N_0 has a very small temperature dependence. It follows that one can estimate the condensed fraction of the stable localized state as $N_0/N \simeq 4/(3N\gamma)$. This estimation is not so rough: choosing for instance $N\gamma = 2$ one finds $N_0/N \simeq 2/3$ in good agreement with the result shown in the upper solid line of Fig. 2 (see where $N_0/N = 0.66$).

In the previous calculations, transverse modes have been neglected and the thermally excited quasi-particles are allowed to populate only the lowest transverse state. This assumption can be justified by a simple argument: In the weakly localized regime (low $N\gamma$) the spectrum of elementary excitations is well approximated by the free Bose gas, where the logitudinal modes have energies $O(\hbar\omega_\perp a_\perp^2/L^2)$ much lower than the $O(\hbar\omega_\perp)$ transverse modes. In this limit we have explicitly verified that, with the chosen parameters ($L/a_\perp = 100$), for $k_B T \lesssim 5\,\hbar\omega_\perp$ the number of quasiparticles in the excited transverse modes is indeed negligible. In the strongly localized region, both longitudinal and transverse low energy excitations are known in the large L limit [6,17], where a finite $O(\hbar\omega_\perp)$ gap separates the two branches. Moreover, our calculations show that for $N\gamma < 4/3$, thermal depletion does not affect deeply the thermodynamics of the model up to the transition temperature.
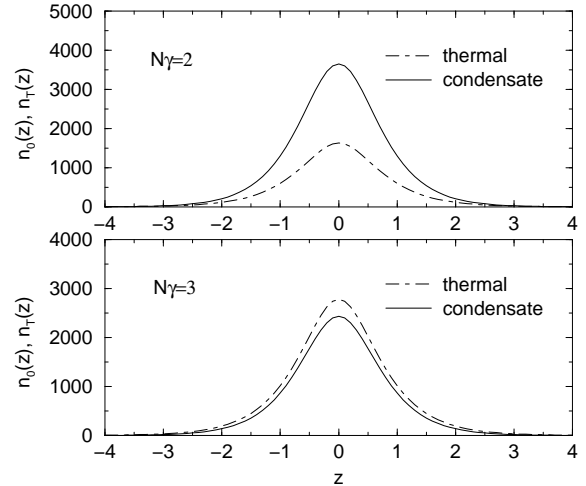

FIG. 3. Azimuthal density profiles of the thermodynamically stable state for $N = 10^4$ atoms with $L/a_\perp = 100$ and $k_B T/(\hbar\omega_\perp) = 2$. Length z is in units of $a_\perp = (\hbar/(m\omega_\perp))^{1/2}$.

For completeness, we have repeated the calculations by using the 1D GPE. Also in this case we have found two localized solutions but the stable one always maintains a condensate fraction close to one, due to the fact that the 1D GPE does not predict the collapse. Thus the

transverse structure of the soliton, taken into account by the NPSE, strongly modifies the thermodynamics of the attractive Bose gas.

In Fig. 3 we plot the density profile $n_0(z)$ of the condensate cloud (solid line) and of the density profile $n_T(z)$ of the thermal cloud (dot-dashed line) for the stable localized state and two values of γ. We have verified that the density profile $n_{out}(z)$ of the quantum depletion reduces by increasing the temperature T and that the quantum depletion N_{out}/N becomes relevant only when the $k_B T$ is of the order of the lowest Bogoliubov energy level. This energy can be easily estimated as $k_B T/(\hbar\omega_\perp) = (\hbar^2/(2m))(2\pi/L)^2/(\hbar\omega_\perp) = 2\pi^2 a_\perp^2/L^2 \simeq 0.002$.
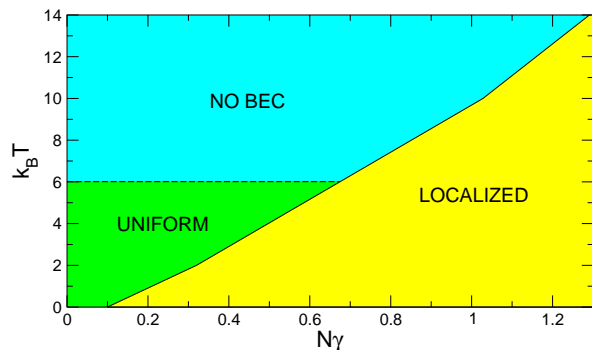

FIG. 4 (color online). Phase diagram in the plane temperature T vs interatomic strength γ for $N = 10^4$ atoms in a toroidal trap, with $L = 100$. The energy $k_B T$ is in units of $\hbar\omega_\perp$ and the length in units of $a_\perp$.

In Fig. 4 we plot the phase diagram of the atomic cloud of bosons in the plane $(N\gamma, T)$ for $L/a_\perp = 100$ and $N = 10^4$. In the figure we insert a dashed line at $k_B T/(\hbar\omega_\perp) = 6.01$, which is the transition temperature T_{BEC} of the Bose-Einstein condensation above which the condensate fraction of the uniform state is zero. The transition temperature T_{BEC} reduces by increasing $L/a_\perp$. In fact, it is easy to show [16] that $k_B T_{BEC}/(\hbar\omega_\perp)$ scales as $Na_\perp^2/L^2$. Fig. 4 displays as a solid line the curve of the uniform-to-localized transition. Remarkably, the BEC transition temperature of the localized solution is much larger than the uniform one. Fig. 4 shows that with $N\gamma > 0.68$, there is a first order transition from localized BEC phase to the the uniform thermal phase without BEC. Instead, for $N\gamma < 0.68$ the no-BEC phase is obtained starting from the uniform phase by increasing the temperature.

In conclusion, we have shown that an attractive Bose condensate in a quasi one-dimensional toroidal trap displays at finite temperature new and intersting features, like the coexistence of a coherent self-bound bright soliton with a thermal cloud, the avoiding of true collapse via population of the out-of-condensate (thermal) component, and the enhancement of the Bose-Einstein transition temperature for the localized solution. We stress

that our predictions can be verified by using a magnetic ring with geometric parameters not too far from those used in Ref. [1] for trapping a repulsive condensate of ^{87}Rb atoms. For instance, a sample of ^{7}Li atoms, which have a negative scattering length ($a_s = -1.4$ nm), can be trapped in a ring with transverse width $a_\perp \simeq 6$ μm, which gives $\hbar\omega_\perp/k_B = \hbar^2/(2a_\perp^2) \simeq 2$ nK. In this way, having $N = 10^4$ atoms the interaction strength is $N\gamma = N2|a_s|/a_\perp \simeq 5$. Then, by taking the azimuthal radius $R = L/(2\pi) \simeq 100$ μm one can test the predictions of Fig. 4 varying the temperature or tuning the scattering length a_s around a Feshbach resonance.

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